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Indexing
&
Abstracting



Irregularity Invariants for Chemical Structures used in the Treatment of COVID-19

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Abstract

The world is going through the pandemic of COVID-19. Remdesivir, chloroquine, hydroxychloroquine and theaflavin are some drugs currently in use for the treatment of the COVID-19 patients. This manuscript aims to compute the irregularity measures for these chemical structures. We believe that our results can be utilized to improve the capacity of these chemical structures.

Keywords: COVID-19, chloroquine, hydroxychloroquine, irregularity indices, remdesivir, theaflavin

Introduction

Historically, the epidemics of influenza and cholera were regarded as the most devastating. Recently, the COVID-19 pandemic which originated from China has affected the health of people all around the world [1]. By September 2020, there were over 32.7 million confirmed cases of COVID-19 including 991,000 deaths. According to WHO, no particular medication for this disease is available. So, it's very important to choose suitable medicine for its treatment. Researchers have tested some chemical compounds [2, 3, 4, 5, 6] and obtained favorable results. These compounds include chloroquine, hydroxylchloroquine, remdesivir (GS5734), and theaflavin.

Molecular graph is a [7, 8] simple graph in which the vertices and edges are considered as the atoms and bonds of the compound, respectively.

Let $G = (V, E)$ be a simple connected graph, where V is the set of vertices and E represents the number of edges present in the graph. The degree of vertex depicts the number of edges attached with that vertex and it is denoted by d_v , where $v \in V(G)$ and e represents an edge $e = uv \in E(G)$. Topological indices (TIs) help us to describe the structure of the graph [9, 10, 11, 12, 13, 14, 15, 16, 17, 18]. The first ever TI was

presented by Wiener in 1947 [19], when he was trying to find out the boiling point of alkanes.

$$W(G) = \sum_{(uv) \subseteq V(G)} d_G(u, v)$$

Gutman, in 1975, presented the definition [20] of Zagreb indices. the oldest degree-based descriptors are two indices known as the first and second Zagreb indices, respectively. The properties of these indices were investigated extensively [21, 22]. These properties can be represented by the mathematical formulae given below.

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v)$$

$$M_2(G) = \sum_{uv \in E(G)} (d_u \times d_v)$$

TI is recognized as an irregularity index [23] if certain conditions are met. Firstly, if the TI of a graph is greater than zero or equal to zero. Secondly, if the TI of a graph is equal to zero, given the graph is regular. Table 1 shows the irregularity indices.

Table 1. Irregularity Indices and their Mathematical Formulae

Irregularity Index	Mathematical Formula
VAR	$\sum_{u \in V} (d_u - \frac{2m}{n})^2 = \frac{M_1(G)}{n} - (\frac{2m}{n})^2$
AL	$\sum_{uv \in E(G)} d_u - d_v $
IR1	$\sum_{u \in V} (d_u)^3 - \frac{2m}{n} \sum_{u \in V} (d_u)^2 = F(G) - \frac{2m}{n} M_1(G)$
IR2	$\sqrt{\frac{\sum_{uv \in E(G)} d_u d_v}{m}} - \frac{2m}{n} = \sqrt{\frac{M_2(G)}{m}} - \frac{2m}{n}$
IRF	$\sum_{uv \in E(G)} (d_u - d_v)^2 = F(G) - 2M_2(G)$
IRFW	$\frac{IRF(G)}{M_2(G)}$

Irregularity Index	Mathematical Formula
IRA	$\sum_{uv \in E(G)} (d_u^{-1/2} - d_v^{-1/2})^2 = n - 2R(G)$
IRB	$\sum_{uv \in E(G)} (d_u^{1/2} - d_v^{1/2})^2 = M_1(G) - 2RR(G)$
IRC	$\frac{\sum_{uv \in E(G)} \sqrt{d_u d_v}}{m} - \frac{2m}{n} = \frac{RR(G)}{m} - \frac{2m}{n}$
IRDIF	$\sum_{uv \in E(G)} \left \frac{d_u}{d_v} - \frac{d_v}{d_u} \right = \sum_{i < j} m_{i,j} \left(\frac{j}{i} - \frac{i}{j} \right)$
IRL	$\sum_{uv \in E(G)} \ln d_u - \ln d_v = \sum_{i < j} m_{i,j} \ln \left(\frac{j}{i} \right)$
IRLU	$\sum_{uv \in E(G)} \frac{ d_u - d_v }{\min(d_u, d_v)} = \sum_{i < j} m_{i,j} \ln \left(\frac{j-i}{i} \right)$
IRLF	$\sum_{uv \in E(G)} \frac{ d_u - d_v }{\sqrt{(d_u d_v)}} = \sum_{i < j} m_{i,j} \left(\frac{j-i}{\sqrt{ij}} \right)$
IRLA	$2 \sum_{uv \in E(G)} \frac{ d_u - d_v }{(d_u + d_v)} = 2 \sum_{i < j} m_{i,j} \left(\frac{j-i}{i+j} \right)$
IRDI	$\sum_{uv \in E(G)} \ln(1 + d_u - d_v) = \sum_{i < j} m_{i,j} \ln(i + j - 1)$
IRGA	$\sum_{uv \in E(G)} \ln \left(\frac{d_u + d_v}{2\sqrt{d_u d_v}} \right) = \sum_{i < j} m_{i,j} \left(\frac{i+j}{2\sqrt{ij}} \right)$

2. Irregularities of the Chemical Structures used for the Treatment of the Patients of COVID-19

In this section, we discuss some chemical structures used for the treatment and management of the patients of COVID-19 by means of the chemical graph theory. We associate these structures with a molecular graph. We can observe from these two-dimensional molecular structures that all of them belong to the family of the irregular graph, so the best way to express these irregularities are irregularity indices. Here, we discuss sixteen irregularity indices for

chloroquine, hydroxychloroquine, remdesivir, and theaflavin in four subsections.

2.1. Irregularity Indices for Remdesivir

This section covers the irregularity indices of remdesivir.

Figure 1 shows the two dimensional molecular graph of remdesivir.

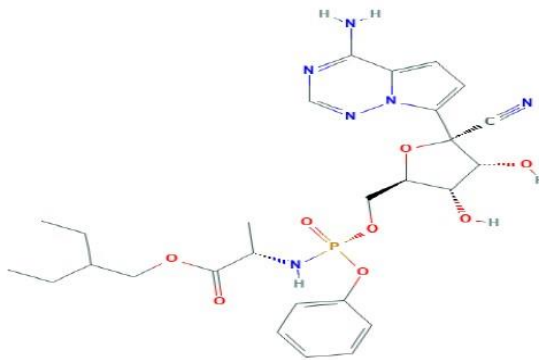


Figure 1. Molecular structure of Remdesivir [24]

The degree-based edge partition of remdesivir is given in Table 2

Table 2. Partition of E (Remdesivir)

(d_u, d_v)	Frequency
(1,2)	2
(1,3)	5
(1,4)	2
(2,2)	9
(2,3)	14
(2,4)	4
(3,3)	6
(3,4)	2

Theorem 2.1. Let's suppose G is the graph of remdesivir. The irregularity indices are as follows:

- (1) $VAR(G) = 13.60$.
- (2) $AL(G) = 42$.

- (3) $IR1(G) = 133.42.$
- (4) $IR2(G) = 0.315.$
- (5) $IRF(G) = 72.$
- (6) $IRFW(G) = 0.280.$
- (7) $IRA(G) = 3.04.$
- (8) $IRB(G) = 7.93.$
- (9) $IRC(G) = -1.67.$
- (10) $IRDIF(G) = 34.76.$
- (11) $IRL(G) = 18.53.$
- (12) $IRLU(G) = 29.66.$ (13) $IRLF(G) = 19.28.$ (14) $IRLA(G) = 17.56.$
- (15) $IRD1(G) = 42.$
- (16) $IRGA(G) = 0.518.$

Proof: Using the edge partition (Table 1), the irregularities of remdesivir are computed as follows:

$$\begin{aligned}
 VAR(G) &= \sum_{u \in V} \left(d_u - \frac{2m}{n} \right)^2 = \frac{M_1(G)}{n} - \left(\frac{2m}{n} \right)^2 \\
 &= \frac{216}{42} - \left(\frac{44}{42} \right)^2 \\
 &= 13.60. \\
 AL(G) &= \sum_{uv \in E(G)} |d_u - d_v| \\
 &= |1 - 2|(2) + |1 - 3|(5) + |1 - 4|(2) + |2 - 2|(9) \\
 &\quad + |2 - 3|(14) + |2 - 4|(4) + |3 - 3|(6) + |3 - 4|(2) \\
 &= 42. \\
 IR1(G) &= \sum_{u \in V} d_u^3 - \frac{2m}{n} \sum_{u \in V} d_u^2 = F(G) - \left(\frac{2m}{n} \right) M_1(G) \\
 &= 586 - \left(\frac{88}{42} \right) 216 \\
 &= 133.42. \\
 IR2(G) &= \sqrt{\frac{\sum_{uv \in E(G)} d_u d_v}{m}} - \frac{2m}{n} = \sqrt{\frac{M_2(G)}{m}} - \frac{2m}{n} \\
 &= \sqrt{\frac{257}{44}} - \frac{2(44)}{42} \\
 &= 0.315.
 \end{aligned}$$

$$\begin{aligned}
 IRF(G) &= \sum_{uv \in E(G)} (d_u - d_v)^2 \\
 &= (1-2)^2(2) + (1-3)^2(5) + (1-4)^2(2) + (2-2)^2(9) \\
 &\quad + (2-3)^2(14) + (2-4)^2(4) + (3-3)^2(6) + (3-4)^2(2) \\
 &= 72.
 \end{aligned}$$

$$\begin{aligned}
 IRFW(G) &= \frac{IRF(G)}{M_2(G)} \\
 &= 0.280.
 \end{aligned}$$

$$\begin{aligned}
 IRA(G) &= \sum_{uv \in E(G)} (d_u^{-1/2} - d_v^{-1/2})^2 = n - 2R(G) \\
 &= (42) - 2(19.48) \\
 &= 3.04.
 \end{aligned}$$

$$\begin{aligned}
 IRB(G) &= \sum_{uv \in E(G)} (d_u^{1/2} - d_v^{1/2})^2 = M_1(G) - 2RR(G) \\
 &= (\sqrt{1} - \sqrt{2})^2 \times 2 + (\sqrt{1} - \sqrt{3})^2 \times 5 + (\sqrt{1} - \sqrt{4})^2 \times 2 + (\sqrt{2} - \sqrt{2})^2 \times 9 \\
 &\quad + (\sqrt{2} - \sqrt{3})^2 \times 14 + (\sqrt{2} - \sqrt{4})^2 \times 9 + (\sqrt{3} - \sqrt{3})^2 \times 6 + (\sqrt{3} - \sqrt{4})^2 \times 9 \\
 &= 7.93.
 \end{aligned}$$

$$\begin{aligned}
 IRC(G) &= \frac{\sum_{uv \in E(G)} \sqrt{d_u d_v}}{m} - \frac{2m}{n} = \frac{RR(G)}{m} - \frac{2m}{n} \\
 &= \frac{18.88}{44} - \left(\frac{88}{42}\right) \\
 &= -1.67.
 \end{aligned}$$

$$\begin{aligned}
 IRDIF(G) &= \sum_{uv \in E(G)} \left| \frac{d_u}{d_v} - \frac{d_v}{d_u} \right| \\
 &= \left| \frac{1}{2} - \frac{2}{1} \right|(2) + \left| \frac{1}{3} - \frac{3}{1} \right|(5) + \left| \frac{1}{4} - \frac{4}{1} \right|(2) + \left| \frac{2}{2} - \frac{2}{2} \right|(9) \\
 &\quad + \left| \frac{2}{3} - \frac{3}{2} \right|(14) + \left| \frac{2}{4} - \frac{4}{2} \right|(4) + \left| \frac{3}{3} - \frac{3}{3} \right|(6) + \left| \frac{3}{4} - \frac{4}{3} \right|(2) \\
 &= 34.76.
 \end{aligned}$$

$$\begin{aligned}
 IRL(G) &= \sum_{uv \in E(G)} |\ln d_u - \ln d_v| \\
 &= |\ln 1 - \ln 2|(2) + |\ln 1 - \ln 3|(5) + |\ln 1 - \ln 4|(2) + |\ln 2 - \ln 2|(9) \\
 &\quad + |\ln 2 - \ln 3|(14) + |\ln 2 - \ln 4|(4) + |\ln 3 - \ln 3|(6) + |\ln 3 - \ln 4|(2) \\
 &= 18.53.
 \end{aligned}$$

$$\begin{aligned}
IRLU(G) &= \sum_{uv \in E(G)} \frac{|d_u - d_v|}{\min(d_u, d_v)} \\
&= \left(\frac{|1-2|}{1}\right)(2) + \left(\frac{|1-3|}{1}\right)(5) + \left(\frac{|1-4|}{1}\right)(2) + \left(\frac{|2-2|}{2}\right)(9) \\
&= \left(\frac{|2-3|}{2}\right)(14) + \left(\frac{|2-4|}{2}\right)(4) + \left(\frac{|3-3|}{3}\right)(6) + \left(\frac{|3-4|}{3}\right)(2) \\
&= 29.66.
\end{aligned}$$

$$\begin{aligned}
IRLF(G) &= \sum_{uv \in E(G)} \frac{|d_u - d_v|}{\sqrt{d_u d_v}} \\
&= \left(\frac{|1-2|}{\sqrt{2}}\right)(2) + \left(\frac{|1-3|}{\sqrt{3}}\right)(5) + \left(\frac{|1-4|}{\sqrt{4}}\right)(2) + \left(\frac{|2-2|}{\sqrt{4}}\right)(9) \\
&= \left(\frac{|2-3|}{\sqrt{6}}\right)(14) + \left(\frac{|2-4|}{\sqrt{8}}\right)(4) + \left(\frac{|3-3|}{\sqrt{9}}\right)(6) + \left(\frac{|3-4|}{\sqrt{12}}\right)(2) \\
&= 19.28.
\end{aligned}$$

$$\begin{aligned}
IRLA(G) &= \sum_{uv \in E(G)} 2 \frac{|d_u - d_v|}{(d_u + d_v)} \\
&= 2 \left(\frac{|1-2|}{1+2}\right)(2) + 2 \left(\frac{|1-3|}{1+3}\right)(5) + 2 \left(\frac{|1-4|}{1+4}\right)(2) + 2 \left(\frac{|2-2|}{2+2}\right)(9) \\
&\quad + 2 \left(\frac{|2-3|}{2+3}\right)(14) + 2 \left(\frac{|2-4|}{2+4}\right)(4) + 2 \left(\frac{|3-3|}{3+3}\right)(6) + 2 \left(\frac{|3-4|}{3+4}\right)(2) \\
&= 17.56.
\end{aligned}$$

$$\begin{aligned}
IRD1(G) &= \sum_{uv \in E(G)} \ln\{1 + |d_u - d_v|\} \\
&= \ln\{1 + |1-2|\}(2) + \ln\{1 + |1-3|\}(5) + \ln\{1 + |1-4|\}(2) + \ln\{1 + |2-2|\}(9) \\
&\quad + \ln\{1 + |2-3|\}(14) + \ln\{1 + |2-4|\}(4) + \ln\{1 + |3-3|\}(6) + \ln\{1 + |3-4|\}(2) \\
&= 42.
\end{aligned}$$

$$\begin{aligned}
IRGA(G) &= \sum_{uv \in E(G)} \ln\left(\frac{d_u + d_v}{2\sqrt{d_u d_v}}\right) \\
&= \ln\left(\frac{1+2}{2\sqrt{1 \times 2}}\right)(2) + \ln\left(\frac{1+3}{2\sqrt{1 \times 3}}\right)(5) + \ln\left(\frac{1+4}{2\sqrt{1 \times 4}}\right)(2) + \ln\left(\frac{2+2}{2\sqrt{2 \times 2}}\right)(9) \\
&\quad + \ln\left(\frac{2+3}{2\sqrt{2 \times 3}}\right)(14) + \ln\left(\frac{2+4}{2\sqrt{2 \times 4}}\right)(4) + \ln\left(\frac{3+3}{2\sqrt{3 \times 3}}\right)(6) + \ln\left(\frac{3+4}{2\sqrt{3 \times 4}}\right)(2) \\
&= 0.518.
\end{aligned}$$

2.2. Irregularity Indices for Chloroquine

This section focuses on the irregularity indices for chloroquine. The two-dimensional molecular graph of chloroquine (Figure 2) has three types of vertices.

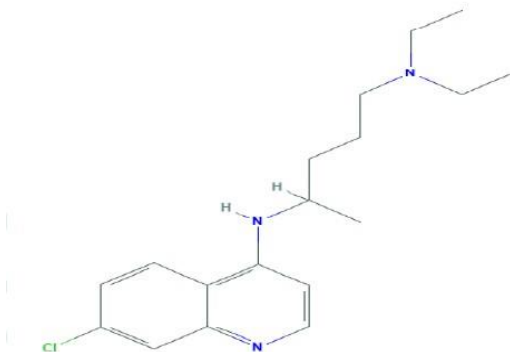


Figure 2. Molecular structure of Chloroquine [25]

Table 3 shows the degree-based edge partition of chloroquine

Table 3. Partition of E (Chloroquine)

(d_u, d_v)	Frequency
(1,2)	2
(1,3)	2
(2,2)	5
(2,3)	12
(3,3)	2

Theorem 2.2. Let's suppose G is the graph of chloroquine. The irregularity indices are as follows:

- (1) $VAR(G) = 0.44$.
- (2) $AL(G) = 18$.
- (3) $IR1(G) = 40.36$.
- (4) $IR2(G) = 0.19$.
- (5) $IRF(G) = 22$.
- (6) $IRFW(G) = 0.183$.
- (7) $IRA(G) = 1$.
- (8) $IRB(G) = 2.623$.
- (9) $IRC(G) = -1.63$.
- (10) $IRDIF(G) = 18.42$.
- (11) $IRL(G) = 8.37$.
- (12) $IRLU(G) = 12$.
- (13) $IRLF(G) = 7.84$.
- (14) $IRLA(G) = 7.13$.

$$(15) IRD1(G) = 11.88.$$

$$(16) IRGA(G) = 16.66.$$

Proof. Using the edge partition of chloroquine given in Table 3, the irregularities of chloroquine are computed as follows:

$$VAR(G) = \sum_{u \in V} \left(d_u - \frac{2m}{n} \right)^2 = \frac{M_1(G)}{n} - \left(\frac{2m}{n} \right)^2$$

$$= \frac{106}{22} - \left(\frac{2(23)}{22} \right)^2$$

$$= 0.44.$$

$$AL(G) = \sum_{uv \in E(G)} |d_u - d_v|$$

$$= |1 - 2|(2) + |1 - 3|(2) + |2 - 2|(5) + |2 - 3|(12) + |3 - 3|(2)$$

$$= 18.$$

$$IR1(G) = \sum_{u \in V} d_u^3 - \left(\frac{2m}{n} \right) \sum_{u \in V} d_u^2 = F(G) - \frac{2m}{n} M_1(G)$$

$$= (262) - \left(\frac{2(23)}{22} \right) (106)$$

$$= 40.36.$$

$$IR2(G) = \sqrt{\frac{\sum_{uv \in E(G)} d_u d_v}{m}} - \frac{2m}{n} = \sqrt{\frac{M_2(G)}{m}} - \frac{2m}{n}$$

$$= \sqrt{\frac{120}{23}} - \frac{2(23)}{22}$$

$$= 0.19.$$

$$IRF(G) = \sum_{uv \in E(G)} (d_u - d_v)^2$$

$$= (1 - 2)^2(2) + (1 - 3)^2(2) + (2 - 2)^2(5) + (2 - 3)^2(12) + (3 - 3)^2(2)$$

$$= 22.$$

$$IRFW(G) = \frac{IRF(G)}{M_2(G)}$$

$$= 0.183.$$

$$IRA(G) = \sum_{uv \in E(G)} (d_u^{-1/2} - d_v^{-1/2})^2 = n - 2R(G)$$

$$= (22) - 2(10.5)$$

$$= 1.$$

$$\begin{aligned}
 IRB(G) &= \sum_{uv \in E(G)} (d_u^{1/2} - d_v^{1/2})^2 = M_1(G) - 2RR(G) \\
 &= (1\sqrt{1} - \sqrt{2})^2(2) + (1\sqrt{1} - \sqrt{3})^2(2)(1\sqrt{2} - \sqrt{2})^2(12) + (1\sqrt{2} - \sqrt{3})^2(12) \\
 &= (1\sqrt{3} - \sqrt{3})^2(2) \\
 &= 2.623.
 \end{aligned}$$

$$\begin{aligned}
 IRC(G) &= \frac{\sum_{uv \in E(G)} \sqrt{d_u d_v}}{m} - \frac{2m}{n} = \frac{RR(G)}{m} - \frac{2m}{n} \\
 &= \frac{10.58}{23} - \frac{46}{22} \\
 &= -1.63.
 \end{aligned}$$

$$\begin{aligned}
 IRDIF(G) &= \sum_{uv \in E(G)} \left| \frac{d_u}{d_v} - \frac{d_v}{d_u} \right| \\
 &= \left| \frac{1}{2} - \frac{2}{1} \right|(2) + \left| \frac{1}{3} - \frac{3}{1} \right|(2) + \left| \frac{2}{2} - \frac{2}{2} \right|(5) \\
 &\quad + \left| \frac{2}{3} - \frac{3}{2} \right|(12) + \left| \frac{3}{3} - \frac{3}{3} \right|(2) \\
 &= 18.42.
 \end{aligned}$$

$$\begin{aligned}
 IRL(G) &= \sum_{uv \in E(G)} |\ln d_u - \ln d_v| \\
 &= |\ln 1 - \ln 2|(2) + |\ln 1 - \ln 3|(2) + |\ln 2 - \ln 2|(5) \\
 &\quad + |\ln 2 - \ln 3|(12) + |\ln 3 - \ln 3|(2) \\
 &= 8.37.
 \end{aligned}$$

$$\begin{aligned}
 IRLU(G) &= \sum_{uv \in E(G)} \frac{|d_u - d_v|}{\min(d_u, d_v)} \\
 &= \left(\frac{|1-2|}{1} \right)(2) + \left(\frac{|1-3|}{1} \right)(2) + \left(\frac{|2-2|}{2} \right)(5) \\
 &\quad + \left(\frac{|2-3|}{2} \right)(12) + \left(\frac{|3-3|}{3} \right)(2) \\
 &= 12.
 \end{aligned}$$

$$\begin{aligned}
 IRLF(G) &= \sum_{uv \in E(G)} \frac{|d_u - d_v|}{\sqrt{d_u \cdot d_v}} \\
 &= \left(\frac{|1-2|}{\sqrt{2}} \right)(2) + \left(\frac{|1-3|}{\sqrt{3}} \right)(2) + \left(\frac{|2-2|}{\sqrt{4}} \right)(5) \\
 &\quad + \left(\frac{|2-3|}{\sqrt{6}} \right)(12) + \left(\frac{|3-3|}{\sqrt{9}} \right)(2) \\
 &= 7.84.
 \end{aligned}$$

$$\begin{aligned}
IRLA(G) &= \sum_{uv \in E(G)} 2 \frac{|d_u - d_v|}{(d_u + d_v)} \\
&= 2 \frac{|1 - 2|}{1 + 2} (2) + 2 \frac{|1 - 3|}{1 + 3} (2) + 2 \frac{|2 - 2|}{2 + 2} (5) \\
&\quad + 2 \frac{|2 - 3|}{2 + 3} (12) + 2 \frac{|3 - 3|}{3 + 3} (2) \\
&= 7.13. \\
IRD1(G) &= \sum_{uv \in E(G)} \ln\{1 + |d_u - d_v|\} \\
&= \ln\{1 + |1 - 2|\} (2) + \ln\{1 + |1 - 3|\} (2) + \ln\{1 + |2 - 2|\} (5) \\
&\quad + \ln\{1 + |2 - 3|\} (12) + \ln\{1 + |3 - 3|\} (2) \\
&= 11.88. \\
IRGA(G) &= \sum_{uv \in E(G)} \ln\left(\frac{d_u + d_v}{2\sqrt{d_u d_v}}\right) \\
&= \ln\left(\frac{1 + 2}{2\sqrt{1 \times 2}}\right) (2) + \ln\left(\frac{1 + 3}{2\sqrt{1 \times 3}}\right) (2) + \ln\left(\frac{2 + 2}{2\sqrt{2 \times 2}}\right) (5) \\
&\quad + \ln\left(\frac{2 + 3}{2\sqrt{2 \times 3}}\right) (12) + \ln\left(\frac{3 + 3}{2\sqrt{3 \times 3}}\right) (2) \\
&= 16.66.
\end{aligned}$$

2.3. Irregularities of Hydroxychloroquine

In this section, irregularity indices for hydroxychloroquine are discussed. The two-dimensional molecular graph of hydroxychloroquine is given in Figure 3. There are three types of vertices present in the graph.

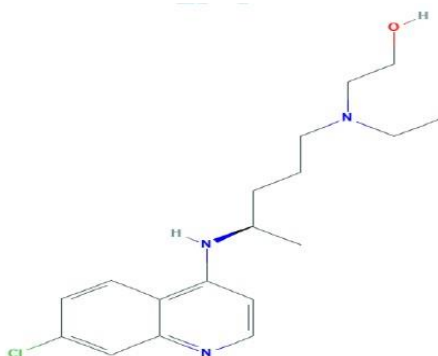


Figure 3. Molecular graph of Hydroxychloroquine [26]

The degree-based edge partition of hydroxychloroquine is given below in Table 4.

Table 4. Partition of E (*Chloroquine*)

(du,dv)	Frequency
(1,2)	2
(1,3)	2
(2,2)	6
(2, 3)	12
(3,3)	2

Theorem 2.3. Let's suppose G is the graph of hydroxychloroquine. The irregularity indices are as follows:

- (1) $VAR(G) = 0.43$.
- (2) $AL(G) = 18$.
- (3) $IR1(G) = 40.43$.
- (4) $IR2(G) = 0.19$.
- (5) $IRF(G) = 22$.
- (6) $IRFW(G) = 0.177$.
- (7) $IRA(G) = 5.78$.
- (8) $IRB(G) = 2.62$.
- (9) $IRC(G) = -1.64$.
- (10) $IRDIF(G) = 18.40$.
- (11) $IRL(G) = 13.29$.
- (12) $IRLU(G) = 12$.
- (13) $IRLF(G) = 8.6$.
- (14) $IRLA(G) = 8.13$.
- (15) $IRD1(G) = 11.88.13$.
- (16) $IRGA(G) = 0.63$.

Proof. Using the edge partition of hydroxychloroquine given in Table 4, the irregularities of hydroxychloroquine are computed as follows:

$$\begin{aligned}
 VAR(G) &= \sum_{u \in V} \left(d_u - \frac{2m}{n} \right)^2 = \frac{M_1(G)}{n} - \left(\frac{2m}{n} \right)^2 \\
 &= \frac{110}{23} - \left(\frac{2(24)}{23} \right)^2 \\
 &= 0.43.
 \end{aligned}$$

$$\begin{aligned}
 AL(G) &= \sum_{uv \in E(G)} |d_u - d_v| \\
 &= |1 - 2|(2) + |1 - 3|(2) + |2 - 2|(6) + |2 - 3|(12) + |3 - 3|(2) \\
 &= 18.
 \end{aligned}$$

$$\begin{aligned}
 IR1(G) &= \sum_{u \in V} d_u^3 - \left(\frac{2m}{n} \right) \sum_{u \in V} d_u^2 = F(G) - \frac{2m}{n} M_1(G) \\
 &= (270) - \left(\frac{2(24)}{23} \right) (110) \\
 &= 40.43.
 \end{aligned}$$

$$\begin{aligned}
 IR2(G) &= \sqrt{\frac{\sum_{uv \in E(G)} d_u d_v}{m}} - \frac{2m}{n} = \sqrt{\frac{M_2(G)}{m}} - \frac{2m}{n} \\
 &= \sqrt{\frac{124}{24}} - \frac{2(24)}{23} \\
 &= 0.19.
 \end{aligned}$$

$$\begin{aligned}
 IRF(G) &= \sum_{uv \in E(G)} (d_u - d_v)^2 \\
 &= (1 - 2)^2(2) + (1 - 3)^2(2) + (2 - 2)^2(6) + (2 - 3)^2(12) + (3 - 3)^2(2) \\
 &= 22.
 \end{aligned}$$

$$\begin{aligned}
 IRFW(G) &= \frac{IRF(G)}{M_2(G)} \\
 &= 0.177.
 \end{aligned}$$

$$\begin{aligned}
 IRA(G) &= \sum_{uv \in E(G)} (d_u^{-1/2} - d_v^{-1/2})^2 = n - 2R(G) \\
 &= (23) - 2(8.61) \\
 &= 5.78.
 \end{aligned}$$

$$\begin{aligned}
 IRB(G) &= \sum_{uv \in E(G)} (d_u^{1/2} - d_v^{1/2})^2 = M_1(G) - 2RR(G) \\
 &= (1\sqrt{1} - \sqrt{2})^2(2) + (1\sqrt{1} - \sqrt{3})^2(2) + (1\sqrt{2} - \sqrt{2})^2(6) \\
 &\quad + (1\sqrt{2} - \sqrt{3})^2(12) + (1\sqrt{3} - \sqrt{3})^2(2) \\
 &= 2.62.
 \end{aligned}$$

$$\begin{aligned}
 IRC(G) &= \frac{\sum_{uv \in E(G)} \sqrt{d_u d_v}}{m} - \frac{2m}{n} = \frac{RR(G)}{m} - \frac{2m}{n} \\
 &= \frac{10.59}{24} - \frac{48}{23} \\
 &= -1.64.
 \end{aligned}$$

$$\begin{aligned}
 IRDIF(G) &= \sum_{uv \in E(G)} \left| \frac{d_u}{d_v} - \frac{d_v}{d_u} \right| \\
 &= \left| \frac{1}{2} - \frac{2}{1} \right| (2) + \left| \frac{1}{3} - \frac{3}{1} \right| (2) + \left| \frac{2}{2} - \frac{2}{2} \right| (6) \\
 &\quad + \left| \frac{2}{3} - \frac{3}{2} \right| (12) + \left| \frac{3}{3} - \frac{3}{3} \right| (2) \\
 &= 18.42.
 \end{aligned}$$

$$\begin{aligned}
 IRL(G) &= \sum_{uv \in E(G)} |\ln d_u - \ln d_v| \\
 &= |\ln 1 - \ln 2| (2) + |\ln 1 - \ln 3| (2) + |\ln 2 - \ln 2| (6) \\
 &\quad + |\ln 2 - \ln 3| (12) + |\ln 3 - \ln 3| (2) \\
 &= 13.29
 \end{aligned}$$

$$\begin{aligned}
 IRLU(G) &= \sum_{uv \in E(G)} \frac{|d_u - d_v|}{\min(d_u, d_v)} \\
 &\quad \left(\frac{|1-2|}{1} \right) (2) + \left(\frac{|1-3|}{1} \right) (2) + \left(\frac{|2-2|}{2} \right) (6) \\
 &\quad + \left(\frac{|2-3|}{2} \right) (12) + \left(\frac{|3-3|}{3} \right) (2) \\
 &= 12
 \end{aligned}$$

$$\begin{aligned}
 IRLF(G) &= \sum_{uv \in E(G)} \frac{|d_u - d_v|}{\sqrt{d_u d_v}} \\
 &= \left(\frac{|1-2|}{\sqrt{2}} \right) (2) + \left(\frac{|1-3|}{\sqrt{3}} \right) (2) + \left(\frac{|2-2|}{\sqrt{4}} \right) (6) + \left(\frac{|2-3|}{\sqrt{6}} \right) (12) + \left(\frac{|3-3|}{\sqrt{9}} \right) (2) \\
 &= 8.6
 \end{aligned}$$

$$\begin{aligned}
IRLA(G) &= \sum_{uv \in E(G)} 2 \frac{|d_u - d_v|}{(d_u + d_v)} \\
&= 2 \frac{|1 - 2|}{1 + 2} (2) + 2 \frac{|1 - 3|}{1 + 3} (2) + 2 \frac{|2 - 2|}{2 + 2} (6) \\
&\quad + 2 \frac{|2 - 3|}{2 + 3} (12) + 2 \frac{|3 - 3|}{3 + 3} (2) \\
&= 8.13. \\
IRD1(G) &= \sum_{uv \in E(G)} \ln\{1 + |d_u - d_v|\} \\
&= \ln\{1 + |1 - 2|\} (2) + \ln\{1 + |1 - 3|\} (2) + \ln\{1 + |2 - 2|\} (6) \\
&\quad + \ln\{1 + |2 - 3|\} (12) + \ln\{1 + |3 - 3|\} (2) \\
&= 11.88. \\
IRGA(G) &= \sum_{uv \in E(G)} \ln\left(\frac{d_u + d_v}{2\sqrt{d_u d_v}}\right) \\
&= \ln\left(\frac{1 + 2}{2\sqrt{1 \times 2}}\right) (2) + \ln\left(\frac{1 + 3}{2\sqrt{1 \times 3}}\right) (2) + \ln\left(\frac{2 + 2}{2\sqrt{2 \times 2}}\right) (6) \\
&\quad + \ln\left(\frac{2 + 3}{2\sqrt{2 \times 3}}\right) (12) + \ln\left(\frac{3 + 3}{2\sqrt{3 \times 3}}\right) (2) \\
&= 16.66.
\end{aligned}$$

2.4. Irregularities of Theaflavin

In this section, irregularity indices for theaflavin are computed. The two-dimensional molecular graph of theaflavin (Figure 4) depicts that three types of vertices are present in the graph.

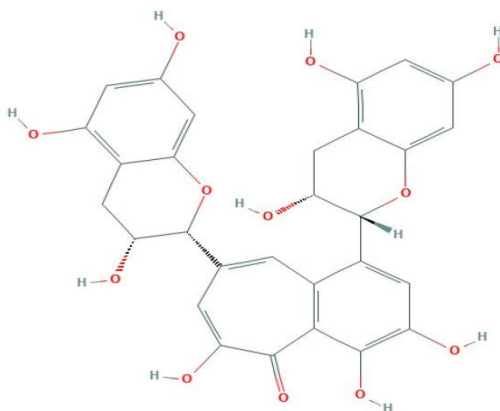


Figure 4. Molecular structure of Theaflavin [27]

Table 5 shows the degree-based edge partition of theaflavin.

Table 5. Partition of E (*Theaflavin*)

(d_u, d_v)	Frequency
(1,3)	10
(2,3)	22
(3,3)	14

Theorem 2.4. Let's suppose G is the graph of theaflavin. The irregularity indices are as follows:

- (1) $VAR(G) = 0.67.$
- (2) $AL(G) = 44.$
- (3) $IR1(G) = 112.92.$
- (4) $IR2(G) = 0.25.$
- (5) $IRF(G) = 62.$
- (6) $IRFW(G) = 0.21.$
- (7) $IRA(G) = 2.18.$
- (8) $IRB(G) = 3.13.$
- (9) $IRC(G) = -2.07.$
- (10) $IRDIF(G) = 45.18.$
- (11) $IRL(G) = 19.78.$
- (12) $IRLU(G) = 31.$
- (13) $IRLF(G) = 20.52.$
- (14) $IRLA(G) = 18.8.$
- (15) $IRD1(G) = 26.22.$
- (16) $IRGA(G) = 1.87.$

Proof. Using the edge partition of theaflavin given in Table 5, the irregularity indices of theaflavin are computed as follows:

$$\begin{aligned}
 VAR(G) &= \sum_{u \in V} \left(d_u - \frac{2m}{n} \right)^2 = \frac{M_1(G)}{n} - \left(\frac{2m}{n} \right)^2 \\
 &= \frac{234}{41} - \left(\frac{2(46)}{41} \right)^2 \\
 &= 0.67.
 \end{aligned}$$

$$\begin{aligned}
 AL(G) &= \sum_{uv \in E(G)} |d_u - d_v| \\
 &= |1 - 3|(10) + |2 - 3|(22) + |3 - 3|(14) \\
 &= 44.
 \end{aligned}$$

$$\begin{aligned}
 IR1(G) &= \sum_{u \in V} d_u^3 - \left(\frac{2m}{n}\right) \sum_{u \in V} d_u^2 = F(G) - \frac{2m}{n} M_1(G) \\
 &= (638) - \left(\frac{2(46)}{41}\right) (234) \\
 &= 112.92.
 \end{aligned}$$

$$\begin{aligned}
 IR2(G) &= \sqrt{\frac{\sum_{uv \in E(G)} d_u d_v}{m}} - \frac{2m}{n} = \sqrt{\frac{M_2(G)}{m}} - \frac{2m}{n} \\
 &= \sqrt{\frac{288}{46}} - \frac{2(46)}{41} \\
 &= 0.25.
 \end{aligned}$$

$$\begin{aligned}
 VAR(G) &= \sum_{u \in V} \left(d_u - \frac{2m}{n}\right)^2 = \frac{M_1(G)}{n} - \left(\frac{2m}{n}\right)^2 \\
 &= \frac{234}{41} - \left(\frac{2(46)}{41}\right)^2 \\
 &= 0.67.
 \end{aligned}$$

$$\begin{aligned}
 AL(G) &= \sum_{uv \in E(G)} |d_u - d_v| \\
 &= |1 - 3|(10) + |2 - 3|(22) + |3 - 3|(14) \\
 &= 44.
 \end{aligned}$$

$$\begin{aligned}
 IR1(G) &= \sum_{u \in V} d_u^3 - \left(\frac{2m}{n}\right) \sum_{u \in V} d_u^2 = F(G) - \frac{2m}{n} M_1(G) \\
 &= (638) - \left(\frac{2(46)}{41}\right) (234) \\
 &= 112.92.
 \end{aligned}$$

$$\begin{aligned}
 IR2(G) &= \sqrt{\frac{\sum_{uv \in E(G)} d_u d_v}{m}} - \frac{2m}{n} = \sqrt{\frac{M_2(G)}{m}} - \frac{2m}{n} \\
 &= \sqrt{\frac{288}{46}} - \frac{2(46)}{41} \\
 &= 0.25.
 \end{aligned}$$

$$\begin{aligned}
 IRF(G) &= \sum_{uv \in E(G)} (d_u - d_v)^2 \\
 &= (1-2)^2(2) + (1-3)^2(2) + (2-2)^2(6) + (2-3)^2(12) + (3-3)^2(2) \\
 &= 62.
 \end{aligned}$$

$$\begin{aligned}
 IRFW(G) &= \frac{IRF(G)}{M_2(G)} \\
 &= 0.21.
 \end{aligned}$$

$$\begin{aligned}
 IRA(G) &= \sum_{uv \in E(G)} (d_u^{-1/2} - d_v^{-1/2})^2 = n - 2R(G) \\
 &= (41) - 2(19.41) \\
 &= 2.18.
 \end{aligned}$$

$$\begin{aligned}
 IRB(G) &= \sum_{uv \in E(G)} (d_u^{1/2} - d_v^{1/2})^2 = M_1(G) - 2RR(G) \\
 &= (1\sqrt{1} - \sqrt{3})^2(10) + (1\sqrt{2} - \sqrt{3})^2(22) + (1\sqrt{3} - \sqrt{3})^2(14) \\
 &= 3.13.
 \end{aligned}$$

$$\begin{aligned}
 IRC(G) &= \frac{\sum_{uv \in E(G)} \sqrt{d_u d_v}}{m} - \frac{2m}{n} = \frac{RR(G)}{m} - \frac{2m}{n} \\
 &= \frac{7.18}{41} - \frac{92}{41} \\
 &= -2.07.
 \end{aligned}$$

$$\begin{aligned}
 IRDIF(G) &= \sum_{uv \in E(G)} \left| \frac{d_u}{d_v} - \frac{d_v}{d_u} \right| \\
 &= \left| \frac{1}{3} - \frac{3}{1} \right|(10) + \left| \frac{2}{3} - \frac{3}{2} \right|(22) + \left| \frac{3}{3} - \frac{3}{3} \right|(14) \\
 &= 45.18.
 \end{aligned}$$

$$\begin{aligned}
 IRL(G) &= \sum_{uv \in E(G)} |\ln d_u - \ln d_v| \\
 &= |\ln 1 - \ln 3|(10) + |\ln 2 - \ln 3|(22) + |\ln 3 - \ln 3|(14) \\
 &= 19.78.
 \end{aligned}$$

$$\begin{aligned}
 IRLU(G) &= \sum_{uv \in E(G)} \frac{|d_u - d_v|}{\min(d_u, d_v)} \\
 &= \left(\frac{|1-3|}{1} \right) (10) + \left(\frac{|2-3|}{2} \right) (22) + \left(\frac{|3-3|}{3} \right) (14) \\
 &= 31
 \end{aligned}$$

$$\begin{aligned}
 IRLF(G) &= \sum_{uv \in E(G)} \frac{|d_u - d_v|}{\sqrt{d_u \cdot d_v}} \\
 &= \left(\frac{|1-3|}{\sqrt{3}} \right) (10) + \left(\frac{|2-3|}{\sqrt{6}} \right) (22) + \left(\frac{|3-3|}{\sqrt{9}} \right) (14) \\
 &= 20.52.
 \end{aligned}$$

$$\begin{aligned}
 IRLA(G) &= \sum_{uv \in E(G)} 2 \frac{|d_u - d_v|}{(d_u + d_v)} \\
 &= 2 \frac{|1-3|}{1+3} (10) + 2 \frac{|2-3|}{2+3} (22) + 2 \frac{|3-3|}{3+3} (14) \\
 &= 18.8.
 \end{aligned}$$

$$\begin{aligned}
 IRD1(G) &= \sum_{uv \in E(G)} \ln\{1 + |d_u - d_v|\} \\
 &= \ln\{1 + |1-3|\} (10) + \ln\{1 + |2-3|\} (22) + \ln\{1 + |3-3|\} (14) \\
 &= 26.22.
 \end{aligned}$$

$$\begin{aligned}
 IRGA(G) &= \sum_{uv \in E(G)} \ln\left(\frac{d_u + d_v}{2\sqrt{d_u d_v}}\right) \\
 &= \ln\left(\frac{1+3}{2\sqrt{1 \times 3}}\right) (10) + \ln\left(\frac{2+3}{2\sqrt{2 \times 3}}\right) (22) + \ln\left(\frac{3+3}{2\sqrt{3 \times 3}}\right) (14) \\
 &= 1.87.
 \end{aligned}$$

3. Conclusion

TIs are very helpful in predicting the physicochemical properties of chemical structures without involving laboratory work. This paper discusses the irregularity indices for chemical structures used in the treatment of COVID-19 namely chloroquine, hydroxychloroquine, remdesivir, and theaflavin. All these chemical structures have an irregular structure, so the best way of predicting their properties is through irregularity indices.

References

- [1] Huang C, Wang Y, Li X, et al. Clinical features of patients infected with 2019 novel coronavirus in Wuhan, China. *Lancet*. 2020 Feb 15;395(10223):497-506. [https://doi.org/10.1016/S0140-6736\(20\)30183-5](https://doi.org/10.1016/S0140-6736(20)30183-5)
- [2] Wang M, Cao R, Zhang L, et al. Remdesivir and chloroquine effectively inhibit the recently emerged novel coronavirus (2019-nCoV) in vitro. *Cell Research*. 2020;30(3):269-71.
- [3] Zhou D, Dai SM, Tong Q. COVID-19: a recommendation to examine the effect of hydroxychloroquine in preventing infection and progression. *J Antimicrobial Chemother*. 2020 Jul 1;75(7):1667-70. <https://doi.org/10.1093/jac/dkaa114>
- [4] Lung J, Lin YS, Yang YH, et al. The potential chemical structure of anti-SARS-CoV-2 RNA-dependent RNA polymerase. *J Med Virol*. 2020 Jun;92(6):693-7. <https://doi.org/10.1002/jmv.25761>
- [5] Liu, W., Morse, J. S., Lalonde, T., & Xu, S. (2020). Learning from the past: possible urgent prevention and treatment options for severe acute respiratory infections caused by 2019-nCoV. *Chembiochem*, 21(5), 730-738.
- [6] Xu X, Chen P, Wang J, et al. Evolution of the novel coronavirus from the ongoing Wuhan outbreak and modeling of its spike protein for risk of human transmission. *Sci China Life Sci*. 2020 Mar;63(3):457-60.
- [7] Klein DJ, Mihalic Z, Plavsic D, et al. Molecular topological index: A relation with the Wiener index. *J Chem Infor Comput Sci*. 1992 Jul;32(4):304-5. <https://doi.org/10.1021/ci00008a008>
- [8] Gutman I, Polansky OE. *Mathematical Concepts in Organic Chemistry*. Springer Science & Business Media; 2012 Dec 6.
- [9] Virk AR. Some New topological invariants for chemical structures used in the treatment of COVID-19 Patients. *Turk J Math Comput Sci*. 2020;12(2):112-119. <https://doi.org/10.47000/tjmcs.730730>
- [10] Virk. A. R., M. A. Rehman & W. Nazeer. (2019). New definition of atomic bond connectivity index to overcome deficiency of structure sensitivity and abruptness in existing definition. *Sci*

- Inquiry Rev.* 2019 Dec 31;3(4):01-20.
<https://doi.org/10.32350/sir.34.01>
- [11] Virk AR. Some Topological Measures for Nicotine. *Earthline J Math Sci.* 2020;4(2):287-296.
- [12] Shao Z, Virk AU, Javed MS, et al. Degree based graph invariants for the molecular graph of Bismuth Tri-Iodide. *Eng Appli Sci Lett.* 2019 Dec;2(1):01-11.
- [13] Bollobás, B., & Erdős, P. (1998). Graphs of extremal weights. *Ars Combinatoria*, 50, 225-233.
- [14] Gao W, Wang W, Farahani MR. Topological indices study of molecular structure in anticancer drugs. *J chem.* 2016 Feb;2016. <https://doi.org/10.1155/2016/3216327>
- [15] Naeem M, Siddiqui MK, Guirao JL, Gao W. New and modified eccentric indices of octagonal grid omni. *Appli Math Nonlinear Sci.* 2018 May 26;3(1):209-28.
- [16] Gao W, Farahani MR, Liu JB. Degree-Based Indices Computation for Special Chemical Molecular and Nanotubes. *Int J Chem Mod.* 2017 Oct 1;9(4):257-68.
- [17] Gao W, Farahani MR, Shi L. Forgotten topological index of some drug structures. *Acta Med Mediterr.* 2016 Jan 1;32(1):579-85.
- [18] Ghorbani M, Ghazi M. Computing some topological indices of triangular benzenoid. *Digest J Nanomater Bios.* 2010 Oct 1;5(4):1107-11.
- [19] Wiener H. Structural determination of paraffin boiling points. *J Am Chem Soci.* 1947 Jan;69(1):17-20. <https://doi.org/10.1021/ja01193a005>
- [20] Yang K, Yu Z, Luo Y, et al. Spatial and temporal variations in the relationship between lake water surface temperatures and water quality-A case study of Dianchi Lake. *Sci Total Environ.* 2018 May 15;624:859-71. <https://doi.org/10.1016/j.scitotenv.2017.12.119>
- [21] Randić, M. (1975). Characterization of molecular branching. *J. Am. Chem. Soc.*, 97 (23), 6609-6615.

- [22] Virk, A. R. (2020). Shingali and Kanabour indices for Bismuth Tri-Iodide *J.Prime Res. Math*, 16(2), 80-88.
- [23] Réti T, Sharafadini R, Dregelyi-Kiss A, et al. Graph irregularity indices used as molecular descriptors in QSPR studies. *MATCH Commun Math Comput Chem*. 2018 Jan 1;79:509-24.
- [24] National Center for Biotechnology Information. PubChem Compound Summary for CID 121304016, Remdesivir. <https://pubchem.ncbi.nlm.nih.gov/compound/Remdesivir>. Accessed Mar. 31, 2021.
- [25] National Center for Biotechnology Information. PubChem Compound Summary for CID 2719, Chloroquine. <https://pubchem.ncbi.nlm.nih.gov/compound/Chloroquine>. Accessed Mar. 31, 2021.
- [26] National Center for Biotechnology Information. PubChem Compound Summary for CID 3652, Hydroxychloroquine. <https://pubchem.ncbi.nlm.nih.gov/compound/Hydroxychloroquine>. Accessed Mar. 31, 2021.
- [27] National Center for Biotechnology Information. PubChem Compound Summary for CID 135403798, Theaflavin. <https://pubchem.ncbi.nlm.nih.gov/compound/Theaflavin>. Accessed Mar. 31, 2021.